

# An introduction to computational algebraic statistics

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## Abstract

In this paper, we introduce the fundamental notion of a Markov basis, which is one of the first connections between commutative algebra and statistics. The notion of a Markov basis is first introduced by Diaconis and Sturmfels ([9]) for conditional testing problems on contingency tables by Markov chain Monte Carlo methods. In this method, we make use of a connected Markov chain over the given conditional sample space to estimate the  $p$  values numerically for various conditional tests. A Markov basis plays an importance role in this arguments, because it guarantees the connectivity of the chain, which is needed for unbiasedness of the estimate, for arbitrary conditional sample space. As another important point, a Markov basis is characterized as generators of the well-specified toric ideals of polynomial rings. This connection between commutative algebra and statistics is the main result of [9]. After this first paper, a Markov basis is studied intensively by many researchers both in commutative algebra and statistics, which yields an attractive field called *computational algebraic statistics*. In this paper, we give a review of the Markov chain Monte Carlo methods for contingency tables and Markov bases, with some fundamental examples. We also give some computational examples by algebraic software Macaulay2 ([11]) and statistical software R. Readers can also find theoretical details of the problems considered in this paper and various results on the structure and examples of Markov bases in [3].

## 1 Conditional tests for contingency tables

A contingency table is a cross-classified table of frequencies. For example, suppose 40 students in some class took examinations of two subjects, Algebra and Statistics. Suppose that both scores are classified to one of the categories, {Excellent, Good, Fair}, and are summarized in Table 1. This is a typical example of two-way contingency tables. Since this table has 3 rows and 3 columns, this is called a  $3 \times 3$  contingency table. The two subjects, Algebra and Statistics, are called *factors* of the table, and the outcomes (i.e., scores) of each factor, {Excellent, Good, Fair}, are called *levels* of each factor. The *cells* of the  $I \times J$  contingency table is the  $IJ$

Table 1: Scores of Algebra and Statistics for 40 students (imaginary data)

Alg\Stat	Excellent	Good	Fair	Total
Excellent	11	5	2	18
Good	4	9	1	14
Fair	2	3	3	8
Total	17	17	6	40

possible combinations of outcomes. Three-way, four-way or higher dimensional contingency tables are defined similarly. For example, adding to the data of Table 1, if the scores of another subject (Geometry, for example) are also given, we have a three-way contingency table. An  $I_1 \times \cdots \times I_m$  ( $m$ -way) contingency table has  $\prod_{i=1}^m I_i$  cells, where  $I_i$  is the number of levels for the  $i$ th factor,  $i = 1, \dots, m$ . In statistical data analysis, the development of methods for analyzing contingency tables began in the 1960s. We refer to [4] for standard textbook in this field.

We begin with simple  $I \times J$  cases, and will consider generalizations to  $m$ -way cases afterward. In statistical inference, we consider underlying random variables and statistical models for observed data such as Table 1, and treat the observed data as one realization of the random variables. In the case of Table 1, it is natural to deal with the two-dimensional discrete random variables

$$(V_1, W_1), (V_2, W_2), \dots, (V_n, W_n), \quad (1)$$

where  $n$  is the *sample size*, ( $n = 40$  for Table 1) and  $(V_k, W_k)$  is the couple of scores obtained by the  $k$ th student. The random couples  $(V_k, W_k)$  for  $k = 1, \dots, n$  are drawn independently from the same distribution

$$P(V_k = i, W_k = j) = \theta_{ij}, \quad i \in [I], j \in [J], k \in [n].$$

Here we use a notation  $[r] = \{1, 2, \dots, r\}$  for  $r \in \mathbb{Z}_{\geq 0}$ , where  $\mathbb{Z}_{\geq 0}$  is the set of nonnegative integers. Note that we use appropriate coding such as 1: Excellent, 2: Good, 3: Fair. The probability  $\theta = (\theta_{ij})$  satisfies the condition

$$\sum_{i=1}^I \sum_{j=1}^J \theta_{ij} = 1,$$

and is called a *parameter*. The parameter space

$$\Delta_{IJ-1} = \left\{ (\theta_{11}, \dots, \theta_{IJ}) \in \mathbb{R}_{\geq 0}^{IJ} : \sum_{i=1}^I \sum_{j=1}^J \theta_{ij} = 1 \right\}$$

is called an  $IJ - 1$  dimensional *probability simplex*.

To consider the data in the form of a contingency table, we also summarize the underlying random variable (1) to the form of the contingency tables as

$$X_{ij} = \sum_{k=1}^n \mathbf{1}(V_k = i, W_k = j),$$

for  $i \in [I], j \in [J]$ , where  $\mathbf{1}(\cdot)$  is the indicator function. By this aggregation from the raw scores to the contingency table, we neglect the order of observations in (1), that is considered to have no information for estimating the parameter  $\theta$ . Then the data  $\mathbf{x} = (x_{ij}) \in \mathbb{Z}_{\geq 0}^{IJ}$  is treated as a realization of  $\mathbf{X} = (X_{ij})$ . The distribution of  $\mathbf{X}$  is a *multinomial distribution* given by

$$p(\mathbf{x}) = P(\mathbf{X} = \mathbf{x}) = \frac{n!}{\prod_{i=1}^I \prod_{j=1}^J x_{ij}!} \prod_{i=1}^I \prod_{j=1}^J \theta_{ij}^{x_{ij}}, \quad \sum_{i=1}^I \sum_{j=1}^J x_{ij} = n. \quad (2)$$

We see that the multinomial distribution (2) is derived from the joint probability function for  $n$  individuals under the assumption that each outcome is obtained independently.

By summarizing the data in the form of contingency tables for fixed sample size  $n$ , the degree of freedom of the observed frequency  $\mathbf{x}$  becomes  $IJ - 1$ , which coincides the degree of freedom of the parameter  $\theta \in \Delta_{IJ-1}$ . Here, we use “degree of freedom” as the number of elements that are free to vary, that is a well-used terminology in statistical fields. We can see the probability simplex  $\Delta_{IJ-1}$  as an example of statistical models, called a *saturated model*. Statistical model is called saturated if the degree of freedom of the parameter equals to the degree of freedom of data.

The saturated model is also characterized as the statistical model having the parameter with the largest degree of freedom. In this sense, the saturated model is the most complex statistical model. In other words, the saturated model is the statistical model that fits the observed data perfectly, i.e., fits the data *without error*. In fact, the parameter  $\theta$  in the saturated model  $\Delta_{IJ-1}$  is estimated from the data as

$$\hat{\theta}_{ij} = \frac{x_{ij}}{n}, \quad i \in [I], \quad j \in [J], \quad (3)$$

that is also called an empirical probability of data. Because we assume that the data  $\mathbf{x}$  is obtained from some probability function such as multinomial distribution (2) *with some randomness*, we want to consider more simple statistical model, i.e., a subset of the saturated model,  $\mathcal{M} \subset \Delta_{IJ-1}$ .

In the two-way contingency tables, a natural, representative statistical model is an *independence model*.

**Definition 1.1.** The independence model for  $I \times J$  contingency tables is the set

$$\mathcal{M}_{indp} = \{\theta \in \Delta_{IJ-1} : \theta_{ij} = \theta_{i+} \theta_{+j}, \forall i, \forall j\}, \quad (4)$$

where

$$\theta_{i+} = \sum_{j=1}^J \theta_{ij}, \quad \theta_{+j} = \sum_{i=1}^I \theta_{ij} \quad \text{for } i \in [I], j \in [J].$$

**Remarks 1.2.** Here we consider that only the sample size  $n$  is fixed. However, several different situations can be considered for  $I \times J$  contingency tables. The situation that we consider here is called a multinomial sampling scheme. For other sampling schemes such as Poisson, binomial and so on, see Chapter 2 of [4] or Chapter 4 of [14]. Accordingly, the corresponding independence model  $\mathcal{M}_{indp}$  is called in different way for other sampling schemes. For example, it is called a *common proportions model* for (product of) binomial sampling scheme where the row sums are fixed, and *main effect model* for Poisson sampling scheme where no marginal is fixed. Though there are also a little differences between the descriptions of these models, we can treat these models almost in the same way by considering the *conditional probability function*, which we consider afterward. Therefore we restrict our arguments to the multinomial sampling scheme in this paper.

There are several equivalent descriptions for the independence model  $\mathcal{M}_{indp}$ . The most common parametric description in statistical textbooks is

$$\mathcal{M}_{indp} = \{\theta \in \Delta_{IJ-1} : \theta_{ij} = \alpha_i \beta_j \text{ for some } (\alpha_i), (\beta_j)\}. \quad (5)$$

For other equivalent parametric descriptions or implicit descriptions, see Section 1 of [17], for example.

The meaning of  $\mathcal{M}_{indp}$  in Table 1 is as follows. If  $\mathcal{M}_{indp}$  is true, there are no relations between the scores of two subjects. Then we can imagine that the scores of two subjects follow the marginal probability functions for each score respectively, and are independent, and the discrepancy we observed in Table 1 is obtained “by chance”. However, it is natural to imagine some structure between the two scores such as “there is a tendency that the students having better scores in Algebra are likely to have better scores in Statistics”, because these subjects are in the same mathematical category. In fact, we see relatively large frequencies 11 and 9 in the diagonals of Table 1, which seem to indicate a positive correlation. Therefore one of natural questions for Table 1 is “Is there some tendency between the two scores that breaks independence?”. To answer this question, we evaluate the fitting of  $\mathcal{M}_{indp}$  by *hypothetical testing*.

The hypothetical testing problem that we consider in this paper is as follows.

$$H_0 : \theta \in \mathcal{M}_{indp} \quad \text{v.s.} \quad H_1 : \theta \in \Delta_{IJ-1} \setminus \mathcal{M}_{indp}.$$

Here we call  $H_0$  a *null hypothesis* and  $H_1$  an *alternative hypothesis*. The terms *null model* and *alternative model* are also used. The hypothetical testing in the above form, i.e., a null model is a subset of a saturated model,  $\mathcal{M} \subset \Delta_{IJ-1}$ , and the alternative model is the complementary set of  $\mathcal{M}$  into the saturated model, is called a *goodness-of-fit test* of model  $\mathcal{M}$ . The testing procedures are composed of steps such as choosing a test statistics, choosing a significance level, and calculating the  $p$  value. We see these steps in order.

**Choosing a test statistic.** First we have to choose a test statistic to use. In general, the term *statistic* means a function of the random variable  $\mathbf{X} = (X_{ij})$ . For example,  $(X_{i+})$  and  $(X_{+j})$  given by

$$X_{i+} = \sum_{j=1}^J X_{ij}, \quad X_{+j} = \sum_{i=1}^I X_{ij} \text{ for } i \in [I], j \in [J]$$

are examples of statistics called the row sums and the column sums, respectively. Other examples of statistics are the row mean  $\bar{X}_{i+} = X_{i+}/J$  and the column mean  $\bar{X}_{+j}/I$  for  $i \in [I], j \in [J]$ . To perform the hypothetical testing, we first select an appropriate statistic, called a *test statistic*, to measure the discrepancy of the observed data from the null model. One of the common test statistic for the goodness-of-fit test is a *Pearson goodness-of-fit*  $\chi^2$  given by

$$\chi^2(\mathbf{X}) = \sum_{i=1}^I \sum_{j=1}^J \frac{(X_{ij} - \hat{m}_{ij})^2}{\hat{m}_{ij}},$$

where  $\hat{m}_{ij}$  is the *fitted value* of  $X_{ij}$  under  $H_0$ , i.e., an estimator of  $E(X_{ij}) = m_{ij} = n\theta_{ij}$ , given by

$$\hat{m}_{ij} = n\hat{\theta}_{ij} = \frac{x_{i+}x_{+j}}{n}. \quad (6)$$

Here we use the *maximum likelihood estimate* of the parameter under the null model,  $\hat{\theta} = (\hat{\theta}_{ij})$ , given by

$$\hat{\theta}_{ij} = \frac{x_{i+}x_{+j}}{n^2}, \quad (7)$$

that is obtained by maximizing the log-likelihood

$$\text{Const} + \sum_{i=1}^I \sum_{j=1}^J x_{ij} \log \theta_{ij}$$

under the constraint  $\theta \in \mathcal{M}_{indp}$ . The meaning of this estimate is also clear in a parametric description (5) since the maximum likelihood estimates of  $(\alpha_i), (\beta_j)$  are given by

$$\hat{\alpha}_i = \frac{x_{i+}}{n}, \quad \hat{\beta}_j = \frac{x_{+j}}{n},$$

respectively. The fitted value for Table 1 under  $\mathcal{M}_{indp}$  is given in Table 2.

There are various test statistics other than the Pearson goodness-of-fit  $\chi^2$  that can be used in our problem. Another representative is the (twice log) likelihood ratio given by

$$2 \sum_{i=1}^I \sum_{j=1}^J X_{ij} \log \frac{X_{ij}}{\hat{m}_{ij}}, \quad (8)$$

where  $\hat{m}_{ij}$  is given by (6). In general, test statistic should be selected by considering their *power*, i.e., the probability that the null hypothesis is rejected if the alternative

Table 2: The fitted value under  $\mathcal{M}_{indp}$  for Table 1

Alg\Stat	Excellent	Good	Fair	Total
Excellent	7.65	7.65	2.70	18
Good	5.95	5.95	2.10	14
Fair	3.40	3.40	1.20	8
Total	17	17	6	40

hypothesis is true. See textbooks such as [15] for the theory of the hypothetical testing, the optimality of the test statistics, examples and the guidelines for choosing test statistics for various problems.

**Choosing a significance level.** Once we choose a test statistic to use, as the Pearson goodness-of-fit  $\chi^2$  for example, the hypothetical testing procedure is written by

$$\chi^2(\mathbf{x}^o) \geq c_\alpha \Rightarrow \text{Reject } H_0,$$

where  $\mathbf{x}^o$  is the observed data, and  $c_\alpha$  is the *critical point at the significance level*  $\alpha$  satisfying

$$P(\chi^2(X) \geq c_\alpha \mid H_0) \leq \alpha. \quad (9)$$

The probability of the left hand side of (9) is called a *type I error*. Equivalently, we define the *p-value* by

$$p = P(\chi^2(X) \geq \chi^2(\mathbf{x}^o) \mid H_0), \quad (10)$$

then the testing procedure is written by

$$p \leq \alpha \Rightarrow \text{Reject } H_0.$$

The meaning of the *p-value* for the data  $\mathbf{x}^o$  is the conditional probability that “more or equally discrepant results are obtained than the observed data if the null hypothesis is true”. Therefore, if *p-value* is significantly small, we conclude that null hypothesis is unrealistic, because it is doubtful that such an extreme result  $\mathbf{x}^o$  is obtained. This is the idea of the statistical hypothetical testing. In this process, the significance level  $\alpha$  plays a threshold to decide the *p-value* is “significantly small” to reject the null hypothesis. In statistical and scientific literature, it is common to choose  $\alpha = 0.05$  or  $\alpha = 0.01$ . Readers can find various topics on *p-value* in [19].

**Calculating the *p-value*.** Once we choose a test statistic and a significance level, all we have to do is to calculate the *p-value* given in (10) for observed data  $\mathbf{x}^o$ . The observed value of the Pearson goodness-of-fit  $\chi^2$  for Table 1 is

$$\chi^2(\mathbf{x}^o) = \sum_{i=1}^3 \sum_{j=1}^3 \frac{(x_{ij}^o - \hat{m}_{ij})^2}{\hat{m}_{ij}} = \frac{(11 - 7.65)^2}{7.65} + \dots + \frac{(3 - 1.20)^2}{1.20} = 8.6687,$$

therefore the  $p$ -value for our  $\mathbf{x}^o$  is

$$p = P(\chi^2(X) \geq 8.6687 \mid H_0).$$

This probability is evaluated based on the *probability function of the test statistic*  $\chi^2(\mathbf{X})$  under  $H_0$ , which we call a *null distribution* hereafter. Unfortunately, the null distribution depends on the unknown parameter  $\theta \in \mathcal{M}_{\text{indp}}$  and the  $p$ -values cannot be calculated in most cases in principle. One naive idea to evaluate the  $p$ -values for such cases is to calculate its supremum in  $\mathcal{M}_{\text{indp}}$  and perform the test as the form

$$\sup_{\theta \in \mathcal{M}_{\text{indp}}} P(\chi^2(X) \geq \chi^2(\mathbf{x}^o) \mid H_0) \leq \alpha \Rightarrow \text{Reject } H_0. \quad (11)$$

However, this idea is hard to implement in general, i.e., it is usually difficult to evaluate the left-hand side of (11) or to seek tests that are powerful under (11). Then, what should we do? We consider the following three strategies for calculating  $p$ -values in this paper.

- (a) Using the asymptotic distribution of the test statistic.
- (b) Exact calculation based on the conditional distribution.
- (c) Estimate the  $p$ -value by the Monte Carlo method.

The aim of this paper is to introduce strategy (c). We will consider each strategy in order.

**(a) Using the asymptotic distribution of the test statistic.** In applications, it is common to rely on various asymptotic theories for the test statistics. As for the Pearson goodness-of-fit test  $\chi^2$  test, the following result is known.

**Theorem 1.3.** *Under the null model  $\mathcal{M}_{\text{indp}}$ , the Pearson goodness-of-fit  $\chi^2(X)$  asymptotically follows the  $\chi^2$  distribution with  $(I-1)(J-1)$  degree of freedom, i.e.,*

$$\lim_{n \rightarrow \infty} P(\chi^2(X) \geq u) = P(V \geq u) \text{ for } u > 0,$$

where  $V \sim \chi^2_{(I-1)(J-1)}$ , i.e.,  $V$  is distributed to the  $\chi^2$  distribution with  $(I-1)(J-1)$  degree of freedom.

This theorem is shown as a consequence of the central limit theorem. In addition, the same asymptotic distribution is given when we consider the conditional limit, i.e., consider  $n \rightarrow \infty$  under the condition that  $X_{i+}/n \rightarrow a_i$  and  $X_{+j}/n \rightarrow b_j$  for  $i \in [I], j \in [J]$  for some fixed  $0 < a_i, b_j < 1$ . See [6] or [18] for detail. Anyway, these asymptotic properties are the reason why we call this test as Pearson goodness-of-fit “ $\chi^2$  test”. Similarly to the Pearson goodness-of-fit  $\chi^2$ , there are several test statistics that have the  $\chi^2$  distribution as the asymptotic distribution. An important example is the likelihood ratio test statistic, which is given in (8) for our setting. Moreover,

several asymptotic good properties of likelihood ratio test statistics are known. See [15] for details. Note also that our methods, Markov chain Monte Carlo methods, can be applicable for arbitrary type of test statistics, though we only consider the Pearson goodness-of-fit  $\chi^2$  in this paper.

Following Theorem 1.3, it is easy to evaluate the asymptotic  $p$ -value of the Pearson goodness-of-fit  $\chi^2$  test. For our data, the observed value of test statistic,  $\chi^2(\mathbf{x}^o) = 8.6687$ , is less than the upper 5 percent point of the  $\chi^2$  distribution with 4 degrees of freedom,  $\chi_{4,0.05}^2 = 9.488$ . Therefore, for the significance level  $\alpha = 0.05$ , we cannot reject the null hypothesis  $H_0$ , i.e., we cannot say that “the fitting of the model  $\mathcal{M}_{indp}$  to Table 1 is poor”. Equivalently, the asymptotic  $p$ -value is calculated as the upper probability of  $\chi_4^2$ , which is 0.0699 and is greater than  $\alpha = 0.05$ . Figure 1 presents the probability density function of the  $\chi_4^2$  distribution. The above results

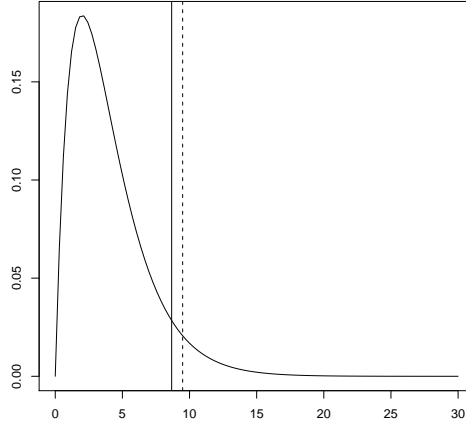


Figure 1:  $\chi^2$  distribution with degree of freedom 4. The vertical solid line indicates the observed value  $\chi^2(\mathbf{x}^o) = 8.6687$ , and the dotted line indicates the critical point for the significance level  $\alpha = 0.05$ ,  $\chi_{4,0.05}^2 = 9.488$ .

can be obtained numerically by the following codes of the statistical software R.

```
> x <- matrix(c(11,5,2,4,9,1,2,3,3), byrow=T, ncol=3, nrow=3)
> x
      [,1] [,2] [,3]
[1,]   11    5    2
[2,]    4    9    1
[3,]    2    3    3
> chisq.test(x)
```

Pearson's Chi-squared test



```

data:  x
X-squared = 8.6687, df = 4, p-value = 0.06994
> pchisq(8.6687,4, lower.tail=F)
[1] 0.06993543
> qchisq(0.05,4,lower.tail=F)          # critical point
[1] 9.487729

```

As we see above, using asymptotic null distribution is easy way to evaluate  $p$ -values, and one of the most common approaches in applications. One of the disadvantages of strategy (a) is that there might not be a good fit with the asymptotic distribution. In fact, because sample size is only  $n = 40$  for Table 1, it is doubtful that we can apply the asymptotic result of  $n \rightarrow \infty$ . Besides, it is well known that there is cases that the fitting of the asymptotic distributions are poor for data with relatively large sample sizes. One such case is sparse data case, another one is unbalanced case. See [12] for these topics.

**(b) Exact calculation based on the conditional distribution.** If we want to avoid asymptotic approaches as strategy (a), an alternative choice is to calculate  $p$ -values *exactly*. For the cases that the null distribution of the test statistics depend on the unknown parameters, we can formulate the exact methods based on the *conditional probability functions* for fixed *minimal sufficient statistics* under the null model  $\mathcal{M}_{indp}$ . The key notion here is the minimal sufficient statistics.

**Definition 1.4.** Let  $\mathbf{X}$  be a discrete random variable with the probability function  $p(\mathbf{x})$  with the parameter  $\theta$ . The statistic  $\mathbf{T}(\mathbf{X})$ , i.e., a vector or a scalar function of  $\mathbf{X}$ , is called sufficient for  $\theta$  if the conditional probability function of  $\mathbf{X}$  for a given  $\mathbf{T}$ ,

$$p(\mathbf{x} \mid \mathbf{t}) = P(\mathbf{X} = \mathbf{x} \mid \mathbf{T}(\mathbf{X}) = \mathbf{t}), \quad (12)$$

does not depend on  $\theta$ . The sufficient statistic  $\mathbf{T}(\mathbf{X})$  is minimal if there is no other sufficient statistics that is a function of  $\mathbf{T}(\mathbf{X})$ .

The meaning of the minimal sufficient statistic is explained as follows. If we know the value of  $\mathbf{T}$ , then knowing  $\mathbf{X}$  provides no further information about the parameter  $\theta$ . Therefore for the parameter estimation or hypothetical testing, it is sufficient to consider the methods based on the minimal sufficient statistic. The minimal sufficient statistics for our two-way problem is as follows.

- Under the saturated model  $\theta \in \Delta_{IJ-1}$ , a minimal sufficient statistic is the contingency table  $\mathbf{X}$ . Adding the additional information such as the scores of the  $k$ th student,  $(V_k, W_k)$ , in (1) gives us no additional information on the estimation of  $\theta$ . Indeed, under the saturated model, the maximum likelihood estimate of the parameter is the empirical probability (3), that is a function of the minimal sufficient statistic.

- Under the independence model  $\mathcal{M}_{indp}$ , a minimal sufficient statistic is the row sums  $\{X_{i+}, i \in [I]\}$  and the column sums  $\{X_{+j}, j \in [J]\}$ , as we see below. Indeed, we have already seen that the maximum likelihood estimate of the parameter under the independence model is (7), that is a function of the row sums and column sums. Note that  $\mathbf{X}$  itself is also the sufficient statistic under the independence model, but is not minimal.

To see that a given statistic  $\mathbf{T}(\mathbf{X})$  is sufficient for a parameter  $\theta$ , a useful way is to rely on the following theorem.

**Theorem 1.5.**  $\mathbf{T}(\mathbf{X})$  is a sufficient statistic for  $\theta$  if and only if the probability function of  $\mathbf{X}$  is factored as

$$p(\mathbf{x}; \theta) = h(\mathbf{x})g(T(\mathbf{x}); \theta), \quad (13)$$

where  $g(\cdot)$  is a function that depends on the parameter  $\theta$  and  $h(\cdot)$  is a function that does not.

For the case of discrete probability function, this theorem, called a *factorization theorem*, is easily (i.e., without measure theories) proved from the definition of the sufficient statistic. Generally, to obtain such a factorization is easier than to compute explicitly the conditional distribution (12). For example, under the parametric description  $\theta_{ij} = \alpha_i \beta_j$ , the probability function of the multinomial distribution (2) is written as

$$p(\mathbf{x}; \theta) = \frac{n!}{\prod_i \prod_j x_{ij}!} \left( \prod_i \alpha_i^{x_{i+}} \right) \left( \prod_j \beta_j^{x_{+j}} \right)$$

and we see that  $T(\mathbf{X}) = (\{X_{i+}\}, \{X_{+j}\})$  is a sufficient statistic for the parameter  $\theta \in \mathcal{M}_{indp}$ .

Here, for later generalization, we introduce a *configuration matrix*  $A$  and express a minimal sufficient statistic by  $A$  as follows. Let the number of the cells of the contingency table  $\mathbf{X}$  be  $p$  and treat  $\mathbf{X}$  as a  $p$ -dimensional column vector. Let  $T(\mathbf{X})$  be a  $d$ -dimensional sufficient statistic for the parameter  $\theta \in \mathcal{M}$ . For example of the independence model  $\mathcal{M}_{indp}$  for  $I \times J$  contingency tables, we have  $\nu = IJ$ ,  $\mathbf{X} = (X_{11}, X_{12}, \dots, X_{IJ})'$  and

$$\mathbf{T}(\mathbf{X}) = (X_{1+}, \dots, X_{I+}, X_{+1}, \dots, X_{+J})'$$

and  $d = I + J$ . Then we see that  $T(\mathbf{X})$  is written as

$$T(\mathbf{X}) = \mathbf{A}\mathbf{X} \quad (14)$$

for  $d \times \nu$  integer matrix  $A$ . For the  $3 \times 3$  contingency tables,  $A$  is written as follows:

$$A = \begin{pmatrix} 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 \\ 1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 \end{pmatrix}. \quad (15)$$

Following the sufficiency of  $T(\mathbf{X}) = A\mathbf{X}$ , the conditional probability function for given  $\mathbf{T} = \mathbf{t}$  does not depend on the parameter. For the case of the independence model  $\mathcal{M}_{indp}$  for two-way contingency tables, it is

$$h(\mathbf{x}) = P(X = \mathbf{x} \mid A\mathbf{X} = \mathbf{t}, H_0) = \frac{\left(\prod_i x_{i+}!\right)\left(\prod_j x_{+j}!\right)}{n! \prod_{i,j} x_{ij}!}, \quad \mathbf{x} \in \mathcal{F}_{\mathbf{t}}, \quad (16)$$

where

$$\mathcal{F}_{\mathbf{t}} = \{\mathbf{x} \in \mathbb{Z}_{\geq 0}^\nu : A\mathbf{x} = \mathbf{t}\}$$

is the conditional sample space, which is called a  $\mathbf{t}$ -*fiber* in the arguments of Markov bases. The conditional probability function  $h(\mathbf{x})$  is called a *hypergeometric distribution*. Using this conditional probability, the conditional  $p$ -value can be defined by

$$p = E_{H_0}(g(\mathbf{X}) \mid A\mathbf{X} = A\mathbf{x}^o) = \sum_{\mathbf{x} \in \mathcal{F}_{A\mathbf{x}^o}} g(\mathbf{x})h(\mathbf{x}) \quad (17)$$

for the observed table  $\mathbf{x}^o$ , where  $g(\mathbf{x})$  is the test function

$$g(\mathbf{x}) = \begin{cases} 1, & \chi^2(\mathbf{x}) \geq \chi^2(\mathbf{x}^o), \\ 0, & \text{otherwise.} \end{cases}$$

Now calculate the conditional  $p$ -value exactly for Table 1. For the observed table  $\mathbf{x}^o$ , i.e., Table 1, we consider the independence model  $\mathcal{M}_{indp}$ . The configuration matrix  $A$  for  $\mathcal{M}_{indp}$  is given in (15). The  $\mathbf{t}$ -fiber including  $\mathbf{x}^o$ , i.e.,  $A\mathbf{x}^o$ -fiber, is the set of all contingency tables that have the same value of the row sums and the column sums to  $\mathbf{x}^o$ ,

$$\mathcal{F}_{A\mathbf{x}^o} = \left\{ \mathbf{x} \in \mathbb{Z}_{\geq 0}^9 : \begin{array}{|c|c|c|c|} \hline x_{11} & x_{12} & x_{13} & 18 \\ \hline x_{21} & x_{22} & x_{23} & 14 \\ \hline x_{31} & x_{32} & x_{33} & 8 \\ \hline 17 & 17 & 6 & 40 \\ \hline \end{array} \right\}.$$

There are 2366 elements in this  $\mathcal{F}_{A\mathbf{x}^o}$ . For each 2366 elements in  $\mathcal{F}_{A\mathbf{x}^o}$ , the conditional probability is given by

$$h(\mathbf{x}) = \frac{(18!14!8!)(17!17!6!)}{40!} \prod_{i,j} \frac{1}{x_{ij}!}, \quad \mathbf{x} \in \mathcal{F}_{A\mathbf{x}^o}.$$

Then we have the exact conditional  $p$ -value

$$p = \sum_{\mathbf{x} \in \mathcal{F}_{A\mathbf{x}^o}} g(\mathbf{x})h(\mathbf{x}) = 0.07035480,$$

where the test function is

$$g(\mathbf{x}) = \begin{cases} 1, & \chi^2(\mathbf{x}) \geq 8.6687, \\ 0, & \text{otherwise.} \end{cases}$$

As a result, we cannot reject  $H_0$  at significance level 0.05, which is the same result to strategy (a).

**Example 1.6.** The following toy example should help the reader in understanding the method. Let consider the  $2 \times 3$  contingency table with the row sums and the column sums given as follows.

$x_{11}$	$x_{12}$	$x_{13}$	3
$x_{21}$	$x_{22}$	$x_{23}$	2
2	2	1	5

There are 5 elements in the fiber as

$$\begin{aligned} \mathcal{F}_{(3,2,2,2,1)} &= \left\{ \begin{bmatrix} 2 & 1 & 0 \\ 0 & 1 & 1 \end{bmatrix}, \begin{bmatrix} 2 & 0 & 1 \\ 0 & 2 & 0 \end{bmatrix}, \begin{bmatrix} 1 & 2 & 0 \\ 1 & 0 & 1 \end{bmatrix}, \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 0 \end{bmatrix}, \begin{bmatrix} 0 & 2 & 1 \\ 2 & 0 & 0 \end{bmatrix} \right\} \\ &= \{\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4, \mathbf{x}_5\}. \end{aligned}$$

The fitted value under the  $\mathcal{M}_{indp}$  is  $\begin{bmatrix} 1.2 & 1.2 & 0.6 \\ 0.8 & 0.8 & 0.4 \end{bmatrix}$ . Then the Pearson goodness-of-fit  $\chi^2$  for each element is calculated as

$$(\chi^2(\mathbf{x}_1), \chi^2(\mathbf{x}_2), \chi^2(\mathbf{x}_3), \chi^2(\mathbf{x}_4), \chi^2(\mathbf{x}_5)) = (2.917, 5, 2.917, 0.833, 5).$$

The conditional probabilities

$$h(\mathbf{x}) = \frac{3!2!2!}{5!} \prod_{i,j} \frac{1}{x_{ij}!} = \frac{2}{5} \prod_{i,j} \frac{1}{x_{ij}!}$$

for each element are calculated as

$$(h(\mathbf{x}_1), h(\mathbf{x}_2), h(\mathbf{x}_3), h(\mathbf{x}_4), h(\mathbf{x}_5)) = (0.2, 0.1, 0.2, 0.4, 0.1).$$

Therefore the conditional  $p$ -value for  $\mathbf{x}_4$  is 1.0, that for  $\mathbf{x}_1$  or  $\mathbf{x}_3$  is 0.6, and that for  $\mathbf{x}_2$  or  $\mathbf{x}_5$  is 0.2.

**Remark 1.7.** We briefly mention the generalization of the above method to general problems and models. First important point is the existence of the minimal sufficient statistics in the form of (14). It is known that, for the *exponential family*, well-known family of the distribution, minimal sufficient statistics exist, and for a special case of the exponential family, called the *toric model*, minimal sufficient statistics of the form (14) exist. The toric model is relatively new concept arising in the field of the computational algebraic statistics and is defined from the configuration matrix  $A = (a_{ij}) \in \mathbb{Z}_{\geq 0}^{d \times \nu}$  as follows. For the  $j$ th column vector  $\mathbf{a}_j = (a_{1j}, \dots, a_{dj})$  of  $A$ ,  $j \in [\nu]$ , define the monomial

$$\theta^{\mathbf{a}_j} = \prod_{i=1}^d \theta_i^{a_{ij}}, \quad j \in [\nu].$$

Then the toric model of  $A$  is the image of the orthant  $\mathbb{R}_{\geq 0}^d$  under the map

$$f : \mathbb{R}^d \rightarrow \mathbb{R}^\nu, \quad \theta \mapsto \frac{1}{\sum_{j=1}^\nu \theta^{\mathbf{a}_j}} (\theta^{\mathbf{a}_1}, \dots, \theta^{\mathbf{a}_\nu}).$$

See Chapter 1.2 of [17] for detail. The toric model specified by the configuration matrix  $A \in \mathbb{Z}_{\geq 0}^{d \times \nu}$  is also written by

$$\mathcal{M}_A = \{\theta = (\theta_i) \in \Delta_{\nu-1} : \log \theta \in \text{rowspan}(A)\},$$

where  $\text{rowspan}(A) = \text{image}(A')$  is the linear space spanned by the rows of  $A$ , and  $\log \theta = (\log \theta_1, \dots, \log \theta_\nu)'$ , where  $'$  is a transpose. In statistical fields, this is called a *log-linear model*. In fact, for example of the independence model  $\mathcal{M}_{\text{indp}}$  of  $2 \times 3$  tables, that is a log-linear model, the parametric description  $\theta_{ij} = \alpha_i \beta_j$  can be written as

$$\begin{pmatrix} \log \theta_{11} \\ \log \theta_{12} \\ \log \theta_{13} \\ \log \theta_{21} \\ \log \theta_{22} \\ \log \theta_{23} \end{pmatrix} = \begin{pmatrix} 1 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \beta_1 \\ \beta_2 \\ \beta_3 \end{pmatrix}.$$

The conditional probability function, i.e., the generalization of the hypergeometric distribution  $h(\mathbf{x})$  in (16) is as follows. For the model specified by the configuration matrix  $A$ , the conditional probability function for given sufficient statistic  $A\mathbf{x}^o$  is

$$P(\mathbf{X} = \mathbf{x} \mid A\mathbf{X} = A\mathbf{x}^o) = C_{A\mathbf{x}^o}^{-1} \frac{1}{\prod_{i \in [\nu]} x_i!},$$

where

$$C_{A\mathbf{x}^o} = \sum_{\mathbf{y} \in \mathcal{F}_{A\mathbf{x}^o}} \frac{1}{\prod_{i \in [\nu]} y_i!} \quad (18)$$

is a normalizing constant. Based on this conditional probability function, we can calculate the conditional  $p$ -values by (17).

Finally, we note an optimality of the method briefly. The conditional procedure mentioned above is justified if we consider the hypothetical testing to the class of *similar tests* and the minimal sufficient statistics is *complete*. For the class of the exponential family, it is known that the minimal sufficient statistic is *complete*. See Chapter 4.3 of [15] for detail.

**(c) Estimate the  $p$ -value by the Monte Carlo method.** The two strategies to evaluate  $p$ -values we have considered, asymptotic evaluation and exact computation, have both advantages and disadvantages. The asymptotic evaluations relying on the

asymptotic  $\chi^2$  distribution are easy to carry out, especially by various packages in softwares such as R. However, poor fitting to the asymptotic distribution can not be ignorable for sparse or unbalanced data even with relatively large sample sizes. The exact calculation of the conditional  $p$ -values is the best method if it is possible to carry out. In fact, various exact methods and algorithms are considered for problems of various types of the contingency tables, statistical models and test statistics. See the survey paper [2] for this field. However, for large size samples, the cardinality of the fiber  $|\mathcal{F}_{A\mathbf{x}^\circ}|$  can exceed billions, making exact computations difficult to be carried out. In fact, it is known that the cardinality of a fiber increases exponentially in the sample size  $n$ . (An approximation for the cardinality of a fiber is given by [10].) For these cases, the Monte Carlo methods can be effective.

The Monte Carlo methods estimate the  $p$ -values as follows. To compute the conditional  $p$ -value (17), generate samples  $\mathbf{x}_1, \dots, \mathbf{x}_N$  from the null distribution  $h(\mathbf{x})$ . Then the  $p$ -value is estimated as  $\hat{p} = \sum_{i=1}^N g(\mathbf{x}_i)/N$ , that is an unbiased estimate of the  $p$ -value. We can set  $N$  according to the performance of our computer. As an advantage of the Monte Carlo method, we can also estimate the accuracy, i.e., *variance* of the estimate. For example, a conventional 95% confidence interval of  $p$ ,  $\hat{p} \pm 1.96\sqrt{\hat{p}(1-\hat{p})/N}$ , is frequently used. The problem here is how to generate samples from the null distribution. We consider *Markov chain Monte Carlo methods*, often abbreviated as the MCMC methods, in this paper.

Following MCMC methods setup, we construct an ergodic Markov chain on the fiber  $\mathcal{F} = \mathcal{F}_{A\mathbf{x}^\circ}$  whose stationary distribution is prescribed, given by (16). Let the elements of  $\mathcal{F}$  be numbered as

$$\mathcal{F} = \{\mathbf{x}_1, \dots, \mathbf{x}_s\}.$$

We write the null distribution on  $\mathcal{F}$  as

$$\pi = (\pi_1, \dots, \pi_s) = (h(\mathbf{x}_1), \dots, h(\mathbf{x}_s)).$$

Here, by standard notation, we treat  $\pi$  as a row vector. We write the transition probability matrix of the Markov chain  $\{Z_t, t \in \mathbb{Z}_{\geq 0}\}$  over  $\mathcal{F}$  as  $Q = (q_{ij})$ , i.e., we define

$$q_{ij} = P(Z_{t+1} = \mathbf{x}_j \mid Z_t = \mathbf{x}_i).$$

Then a probability distribution  $\theta \in \Delta_{s-1}$  is called a stationary distribution if it satisfies  $\theta = \theta Q$ . The stationary distribution uniquely exists if the Markov chain is irreducible, (i.e., connected in this case) and aperiodic. Therefore for the connected and aperiodic Markov chain, starting from an arbitrary state  $Z_0 = \mathbf{x}_i$ , the distribution of  $Z_t$  for large  $t$  is close to its stationary distribution. If we can construct a connected and aperiodic Markov chain with the stationary distribution  $\pi$ , by running the Markov chain and discarding a large number  $t$  of initial steps (called *burn-in steps*), we can treat  $Z_{t+1}, Z_{t+2}, \dots$  to be samples from the null distribution  $\pi$  and use them to estimate  $p$ -values. Then the problem becomes *how to construct a connected and aperiodic Markov chain with the stationary distribution as the null*

distribution  $\pi$  over  $\mathcal{F}$ . Among these conditions, the conditions for the stationary distribution can be solved easily. Once we construct an arbitrary connected chain over  $\mathcal{F}$ , we can modify its stationary distribution to the given null distribution  $\pi$  as follows.

**Theorem 1.8** (Metropolis-Hastings algorithm). *Let  $\pi$  be a probability distribution on  $\mathcal{F}$ . Let  $R = (r_{ij})$  be the transition probability matrix of a connected, aperiodic and symmetric Markov chain over  $\mathcal{F}$ . Then the transition probability matrix  $Q = (q_{ij})$  defined by*

$$\begin{aligned} q_{ij} &= r_{ij} \min \left( 1, \frac{\pi_j}{\pi_i} \right), \quad i \neq j \\ q_{ii} &= 1 - \sum_{j \neq i} q_{ij} \end{aligned}$$

satisfies  $\pi = \pi Q$ .

This theorem is a special case of [13]. Though the symmetry assumption ( $r_{ij} = r_{ji}$ ) can be removed easily, we only consider symmetric  $R$  for simplicity. The proof of this theorem is easy and is omitted. See [13] or Chapter 4.1 of [14], for example. Instead, we consider the algorithm for data of small size.

**Example 1.9.** Consider the small example in Example 1.6. As we have seen, the fiber is

$$\mathcal{F} = \{\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4, \mathbf{x}_5\}$$

and the null distribution is

$$\pi = (\pi_1, \dots, \pi_5) = (h(\mathbf{x}_1), \dots, h(\mathbf{x}_5)) = (0.2, 0.1, 0.2, 0.4, 0.1).$$

Using the Markov basis we consider in the next section, we can construct a connected, aperiodic and symmetric Markov chain with the transition probability matrix

$$R = \begin{pmatrix} 1/2 & 1/6 & 1/6 & 1/6 & 0 \\ 1/6 & 2/3 & 0 & 1/6 & 0 \\ 1/6 & 0 & 1/2 & 1/6 & 1/6 \\ 1/6 & 1/6 & 1/6 & 1/3 & 1/6 \\ 0 & 0 & 1/6 & 1/6 & 2/3 \end{pmatrix}. \quad (19)$$

Following Theorem 1.8, we modify the Markov chain to have the transition probability matrix

$$Q = \begin{pmatrix} 7/12 & 1/12 & 1/6 & 1/6 & 0 \\ 1/6 & 2/3 & 0 & 1/6 & 0 \\ 1/6 & 0 & 7/12 & 1/6 & 1/12 \\ 1/12 & 1/24 & 1/12 & 3/4 & 1/24 \\ 0 & 0 & 1/6 & 1/6 & 2/3 \end{pmatrix}.$$

We can check that the eigenvector from the left of  $Q$  with the eigenvalue 1 is  $\pi$ . We can also check that each row vector of  $Q^T$  for large  $T$  converges to  $\pi$ .

An important advantage of the Markov chain Monte Carlo method is that it does not require the explicit evaluation of the normalizing constant of the null distribution. As is shown in Theorem 1.8, we only need to know  $\pi$  up to a multiplicative constant, because the normalizing constant, (18) in the general form, canceled in the ratio  $\pi_j/\pi_i$ . With Theorem 1.8, the remaining problem is to construct an arbitrary connected and aperiodic Markov chain over  $\mathcal{F}$ , that is solved by the Gröbner basis theory.

## 2 Markov bases and ideals

As stated in the previous section, the main task for estimating  $p$ -values thanks to MCMC methods is to construct a connected and aperiodic Markov chain over  $\mathcal{F} = \mathcal{F}_{A\mathbf{x}^o}$  with stationary distribution given by (16). Here,  $A \in \mathbb{Z}^{d \times \nu}$  is a given configuration matrix,  $\mathbf{x}^o \in \mathbb{Z}_{\geq 0}^\nu$  is the observed contingency table and  $\mathcal{F}_{A\mathbf{x}^o}$ , a  $A\mathbf{x}^o$ -fiber, is the set of all contingency tables with the same value of the minimal sufficient statistics to  $\mathbf{x}^o$ ,

$$\mathcal{F}_{A\mathbf{x}^o} = \{\mathbf{x} \in \mathbb{Z}_{\geq 0}^\nu : A\mathbf{x} = A\mathbf{x}^o\}.$$

We write the integer kernel of  $A$  as

$$\text{Ker}_{\mathbb{Z}}(A) = \text{Ker}(A) \cap \mathbb{Z}^\nu = \{\mathbf{z} \in \mathbb{Z}^\nu : A\mathbf{z} = \mathbf{0}\}.$$

An element of  $\text{Ker}_{\mathbb{Z}}(A)$  is called a *move*. Note that  $\mathbf{x} - \mathbf{y} \in \text{Ker}_{\mathbb{Z}}(A)$  if and only if  $\mathbf{x}, \mathbf{y} \in \mathcal{F}_{A\mathbf{x}^o}$ . Then for a given subset  $\mathcal{B} \subset \text{Ker}_{\mathbb{Z}}(A)$  and  $\mathbf{t} \in \mathbb{Z}_{\geq 0}^d$ , we can define undirected graph  $G_{\mathbf{t}, \mathcal{B}} = (V, E)$  by

$$V = \mathcal{F}_{\mathbf{t}}, \quad E = \{(\mathbf{x}, \mathbf{y}) : \mathbf{x} - \mathbf{y} \in \mathcal{B} \text{ or } \mathbf{y} - \mathbf{x} \in \mathcal{B}\}.$$

**Definition 2.1** (A Markov basis).  $\mathcal{B} \subset \text{Ker}_{\mathbb{Z}}(A)$  is a Markov basis for  $A$  if  $G_{\mathbf{t}, \mathcal{B}}$  is connected for arbitrary  $\mathbf{t} \in \mathbb{Z}_{\geq 0}^d$ .

Once we obtain a Markov basis  $\mathcal{B}$  for  $A$ , we can construct a connected Markov chain over  $\mathcal{F}_{A\mathbf{x}^o}$  easily as follows. For each state  $\mathbf{x} \in \mathcal{F}_{A\mathbf{x}^o}$ , randomly choose a move  $\mathbf{z} \in \mathcal{B}$  and a sign  $\varepsilon \in \{-1, 1\}$  and consider  $\mathbf{x} + \varepsilon\mathbf{z}$ . If  $\mathbf{x} + \varepsilon\mathbf{z} \in \mathcal{F}_{A\mathbf{x}^o}$ , then  $\mathbf{x} + \varepsilon\mathbf{z}$  is the next state, otherwise stay at  $\mathbf{x}$ . Then we have the connected Markov chain over  $A\mathbf{x}^o$ . We see these arguments in an example.

**Example 2.2.** Again we consider a small data of Example 1.6, where the fiber is redisplayed below.

$$\begin{aligned} \mathcal{F}_{(3,2,2,2,1)} &= \left\{ \begin{bmatrix} 2 & 1 & 0 \\ 0 & 1 & 1 \end{bmatrix}, \begin{bmatrix} 2 & 0 & 1 \\ 0 & 2 & 0 \end{bmatrix}, \begin{bmatrix} 1 & 2 & 0 \\ 1 & 0 & 1 \end{bmatrix}, \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 0 \end{bmatrix}, \begin{bmatrix} 0 & 2 & 1 \\ 2 & 0 & 0 \end{bmatrix} \right\} \\ &= \{\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4, \mathbf{x}_5\}. \end{aligned}$$



The integer kernel for the configuration matrix

$$A = \begin{pmatrix} 1 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 1 \\ 1 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 1 \end{pmatrix} \quad (20)$$

includes moves such as

$$\mathbf{z}_1 = \begin{bmatrix} 1 & -1 & 0 \\ -1 & 1 & 0 \end{bmatrix}, \quad \mathbf{z}_2 = \begin{bmatrix} 1 & 0 & -1 \\ -1 & 0 & 1 \end{bmatrix}, \quad \mathbf{z}_3 = \begin{bmatrix} 0 & 1 & -1 \\ 0 & -1 & 1 \end{bmatrix}, \quad \begin{bmatrix} 2 & -1 & -1 \\ -2 & 1 & 1 \end{bmatrix}, \quad \dots$$

From these, we consider some sets of moves. If we consider  $\mathcal{B}_1 = \{\mathbf{z}_1\}$ , corresponding undirected graph  $G_{(3,2,2,2,1),\mathcal{B}_1}$  is given in Figure 2(a), which is not connected. Therefore  $\mathcal{B}_1$  is not a Markov basis. If we consider  $\mathcal{B}_2 = \{\mathbf{z}_1, \mathbf{z}_2\}$ , corresponding undirected graph  $G_{(3,2,2,2,1),\mathcal{B}_2}$  is given in Figure 2(b), which is connected. However,  $\mathcal{B}_2$  is also not a Markov basis, because there exists  $\mathbf{t} \in \mathbb{Z}_{\geq 0}^5$  where  $G_{\mathbf{t},\mathcal{B}_2}$  is not connected. An example of such  $\mathbf{t}$  is  $\mathbf{t} = (1, 1, 0, 1, 1)$ , with the corresponding  $\mathbf{t}$ -fiber is a two-element set

$$\mathcal{F}_{(1,1,0,1,1)} = \left\{ \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} \right\}. \quad (21)$$

The above example shows that a Markov basis includes  $\mathbf{z}_3$  to connect the two elements above. In fact,  $\mathcal{B} = \{\mathbf{z}_1, \mathbf{z}_2, \mathbf{z}_3\}$  is a Markov basis for this  $A$ , with the corresponding undirected graph  $G_{(3,2,2,2,1),\mathcal{B}_3}$  in Figure 2(c). The transition probability

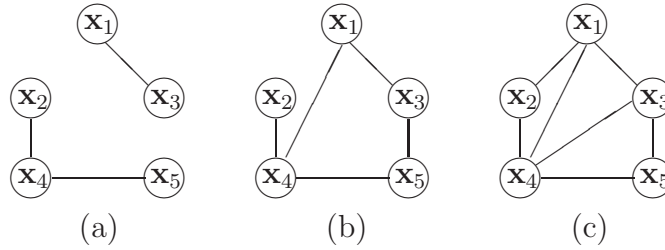


Figure 2: Undirected graphs for  $\mathcal{B}_1, \mathcal{B}_2, \mathcal{B}_3$  for  $\mathbf{t} = (3, 2, 2, 2, 1)$ .

matrix (19) in Example 1.9 corresponds to a Markov chain constructed from  $\mathcal{B}_3$  as “in each step, choose 3 elements in  $\mathcal{B}_3$  and its sign  $\{-1, 1\}$  with equal probabilities”.

At first sight, we may feel the cases such as (21) are trivial and may imagine that “if we only consider the cases with  $\mathbf{t} \in \mathbb{Z}_{>0}^d$ , i.e., cases with strictly positive minimal sufficient statistics (that may be realistic situations in the actual data analysis), it is easy to connect the fiber  $\mathcal{F}_{\mathbf{t}}$ ”. However, it is not so. We will see an example where complicated moves are needed even for the fiber with positive  $\mathbf{t}$ .

The connection between the Markov basis and a *toric ideal* of a polynomial ring by [9] is as follows. Let  $k[\mathbf{u}] = k[u_1, u_2, \dots, u_\nu]$  denote the ring of polynomials in  $\nu$  variables over a field  $k$ . Let a contingency table  $\mathbf{x} \in \mathbb{Z}_{\geq 0}^\nu$  be mapped to the monomial  $\mathbf{u}^{\mathbf{x}} \in k[\mathbf{u}]$ , and a move, i.e., an element of the integer kernel  $\mathbf{z} = \mathbf{z}^+ - \mathbf{z}^- \in \text{Ker}_{\mathbb{Z}}(A)$ , be mapped to the binomial  $\mathbf{u}^{\mathbf{z}^+} - \mathbf{u}^{\mathbf{z}^-} \in k[\mathbf{u}]$ . For the case of the independence model for the  $3 \times 3$  contingency tables, examples of these correspondences are as follows.

$$\begin{array}{|c|c|c|} \hline 11 & 5 & 2 \\ \hline 4 & 9 & 1 \\ \hline 2 & 3 & 3 \\ \hline \end{array} \iff u_{11}^{11} u_{12}^5 u_{13}^2 u_{21}^4 u_{22}^9 u_{23}^2 u_{31}^3 u_{32}^3 u_{33}^3$$

$$\begin{array}{|c|c|c|} \hline 2 & -1 & -1 \\ \hline -3 & 1 & 2 \\ \hline 1 & 0 & -1 \\ \hline \end{array} \iff u_{11}^2 u_{22} u_{23}^2 u_{31} - u_{12} u_{13} u_{21}^3 u_{33}$$

The binomial ideal in  $k[\mathbf{u}]$  generated by the set of binomials corresponding to the set of moves for  $A$ ,

$$I_A = \left\langle \left\{ \mathbf{u}^{\mathbf{z}^+} - \mathbf{u}^{\mathbf{z}^-} : \mathbf{z}^+ - \mathbf{z}^- \in \text{Ker}_{\mathbb{Z}}(A) \right\} \right\rangle,$$

is the *toric ideal* of configuration  $A$ .

**Theorem 2.3** (Theorem 3.1 of [9]).  $\mathcal{B} = \{\mathbf{z}_1, \dots, \mathbf{z}_L\} \subset \text{Ker}_{\mathbb{Z}}(A)$  is a Markov basis for  $A$  if and only if  $\{\mathbf{u}^{\mathbf{z}_i^+} - \mathbf{u}^{\mathbf{z}_i^-} : i = 1, \dots, L\}$  generates  $I_A$ .

A proof of Theorem 2.3 is given in the original paper [9]. We can also find more detailed proof in Chapter 4 of [14]. In these proofs, the sufficiency and the necessity are shown by induction on some integer. In the proof of sufficiency, this integer represents the number of steps of the chain, and the argument is straightforward. On the other hand, in the proof of necessity, this integer represents the number of terms in the expansion that we want to show in the proof, and is not necessarily equal to the number of steps of the chain. Theorem 2.3 shows a non-trivial result on this point.

To calculate a Markov basis for a given configuration matrix  $A$ , we can use the *elimination theory*. For this purpose, we also prepare variables  $\mathbf{v} = \{v_1, \dots, v_d\}$  for the minimal sufficient statistic  $\mathbf{t}$  and consider the polynomial ring  $k[\mathbf{v}] = k[v_1, \dots, v_d]$ . The relation  $\mathbf{t} = A\mathbf{x}$  can be expressed by the homomorphism

$$\begin{aligned} \psi_A : k[\mathbf{u}] &\rightarrow k[\mathbf{v}] \\ u_j &\mapsto v_1^{a_{1j}} v_2^{a_{2j}} \dots v_d^{a_{dj}}. \end{aligned}$$

Then the toric ideal  $I_A$  is also expressed as  $I_A = \text{Ker}(\psi_A)$ . We now have the following.

**Corollary 2.4** (Theorem 3.2 of [9]). Let  $I_A^*$  be the ideal of  $k[\mathbf{u}, \mathbf{v}]$  given by

$$I_A^* = \langle -\psi_A(u_j) + v_j, j = 1, \dots, \nu \rangle \subset k[\mathbf{u}, \mathbf{v}].$$

Then we have  $I_A = I_A^* \cap k[\mathbf{u}]$ .

Corollary 2.4 suggests that we can obtain a generator of  $I_A$  as its Gröbner basis for an appropriate term order called an elimination order. For an ideal  $J \in k[\mathbf{u}]$  and a term order  $\prec$ , a set of polynomials  $\{g_1, \dots, g_s\}$ ,  $g_1, \dots, g_s \in J$ , is called a Gröbner basis of  $I$  with respect to a term order  $\prec$ , if  $\{\text{in}_\prec(g_1), \dots, \text{in}_\prec(g_s)\}$  generates an initial ideal of  $J$  defined by  $\text{in}_\prec(J) = \langle \{\text{in}_\prec(f) : 0 \neq f \in J\} \rangle$ . Here we write  $\text{in}_\prec(f)$  as an initial term of  $f$  with respect to a term order  $\prec$ . For more theories and results on Gröbner bases, see textbooks such as [7]. The elimination theory is one of the useful applications of Gröbner bases and is used for our problem as follows. For the reduced Gröbner basis  $G^*$  of  $I_A^*$  for any term order satisfying  $\{v_1, \dots, v_d\} \succ \{u_1, \dots, u_\nu\}$ ,  $G^* \cap k[\mathbf{u}]$  is a reduced Gröbner basis of  $I_A$ . Because the Gröbner basis is a generator of  $I_A$ , we can obtain a Markov basis for  $A$  as the reduced Gröbner basis in this way.

The computations of Gröbner bases can be carried out by various algebraic softwares such as Macaulay2 ([11]), SINGULAR ([8]), CoCoA ([5]), Risa/Asir ([16]) and 4ti2 ([1]). Here, we show some computations by Macaulay2, because we can also rapidly use it online at the website <sup>1</sup>. We start with a simple example.

**Example 2.5.** In Example 2.2, we give a Markov basis for the independence model for  $2 \times 3$  contingency tables without any proof or calculations. Here we check that the set of 3 moves

$$\left\{ \mathbf{z}_1 = \begin{array}{|c|c|c|} \hline 1 & -1 & 0 \\ \hline -1 & 1 & 0 \\ \hline \end{array}, \mathbf{z}_2 = \begin{array}{|c|c|c|} \hline 1 & 0 & -1 \\ \hline -1 & 0 & 1 \\ \hline \end{array}, \mathbf{z}_3 = \begin{array}{|c|c|c|} \hline 0 & 1 & -1 \\ \hline 0 & -1 & 1 \\ \hline \end{array} \right\}$$

constitute a Markov basis for  $A$  given in (20). In other words, we check that the corresponding toric ideal  $I_A$  is generated by 3 binomials

$$\{u_{11}u_{22} - u_{12}u_{21}, u_{11}u_{23} - u_{13}u_{21}, u_{12}u_{23} - u_{13}u_{22}\}. \quad (22)$$

Following Corollary 2.4, we prepare the variable  $\mathbf{v} = (v_1, \dots, v_5)$  for the row sums and column sums of  $\mathbf{x}$  as

$$\begin{array}{|c|c|c|} \hline x_{11} & x_{12} & x_{13} \\ \hline x_{21} & x_{22} & x_{23} \\ \hline \end{array} \begin{array}{l} v_1 \\ v_2 \end{array}$$

$$\begin{array}{ccc} v_3 & v_4 & v_5 \end{array}$$

and consider the homomorphism

$$\begin{aligned} u_{11} &\mapsto v_1v_3, & u_{12} &\mapsto v_1v_4, & u_{13} &\mapsto v_1v_5, \\ u_{21} &\mapsto v_2v_3, & u_{22} &\mapsto v_2v_4, & u_{23} &\mapsto v_2v_5. \end{aligned}$$

Then under the elimination order  $\mathbf{v} \succ \mathbf{u}$ , compute the reduced Gröbner basis of the toric ideal

$$I_A^* = \langle -v_1v_3 + u_{11}, -v_1v_4 + u_{12}, \dots, -v_2v_5 + u_{23} \rangle.$$

These calculations are done by Macaulay2 as follows.

---

<sup>1</sup>Macaulay2 online: <http://habanero.math.cornell.edu.3690>

```

i1 : R=QQ[v1,v2,v3,v4,v5,u11,u12,u13,u21,u22,u23,MonomialOrder=>{5,6}]

o1 = R

o1 : PolynomialRing

i2 : I=ideal(-v1*v3+u11,-v1*v4+u12,-v1*v5+u13,-v2*v3+u21,-v2*v4+u22,-v2*v5+u23)

o2 = ideal (- v1*v3 + u11, - v1*v4 + u12, - v1*v5 + u13, - v2*v3 + u21, - v2*v4
-----
+ u22, - v2*v5 + u23)

o2 : Ideal of R

i3 : G=gb(I); g=gens(G)

o4 = | u13u22-u12u23 u13u21-u11u23 u12u21-u11u22 v4u23-v5u22 v4u13-v5u12
-----
v3u23-v5u21 v3u22-v4u21 v3u13-v5u11 v3u12-v4u11 v1u23-v2u13 v1u22-v2u12
-----
v1u21-v2u11 v2v5-u23 v1v5-u13 v2v4-u22 v1v4-u12 v2v3-u21 v1v3-u11 |

o4 : Matrix R <--- R

i5 : selectInSubring(1,g)

o5 = | u13u22-u12u23 u13u21-u11u23 u12u21-u11u22 |

o5 : Matrix R <--- R

```

The output `o4` shows the reduced Gröbner basis of  $I_A^*$  under the elimination (reverse lexicographic) order  $\mathbf{v} \succ \mathbf{u}$ , and the output `o5` shows the reduced Gröbner basis of  $I_A$ , which we can use as a Markov basis. We have now checked a Markov basis (22).

From the Markov basis (22), we may imagine that the set of moves corresponding to the binomials

$$\{u_{ij}u_{i'j'} - u_{ij'}u_{i'j}, \quad 1 \leq i < i' \leq I, \quad 1 \leq j < j' \leq J\}$$

forms a Markov basis for the independence model of the  $I \times J$  contingency tables, which is actually true. This fact is given and proved as Theorem 2.1 of [3], for example.

Now we are ready to estimate  $p$ -value for our original problem of  $3 \times 3$  contingency table in Table 1. The Markov basis for this problem is formed by 9 moves of the above type. Using this Markov basis, we calculate the conditional  $p$ -values for Table 1 by the Markov chain Monte Carlo method. For each step of the chain, we choose an element of the Markov basis randomly, and modify the transition probability by

Theorem 1.8. We start the chain at the observed table  $\mathbf{x}^o$  of Table 1, discard initial 50000 steps as the burn-in steps, and have 100000 samples of the Pearson goodness-of-fit  $\chi^2$ . Figure 3 is a histogram of the sampled Pearson goodness-of-fit  $\chi^2$  with the asymptotic  $\chi_4^2$  distribution. In these 100000 samples, 6681 samples are larger

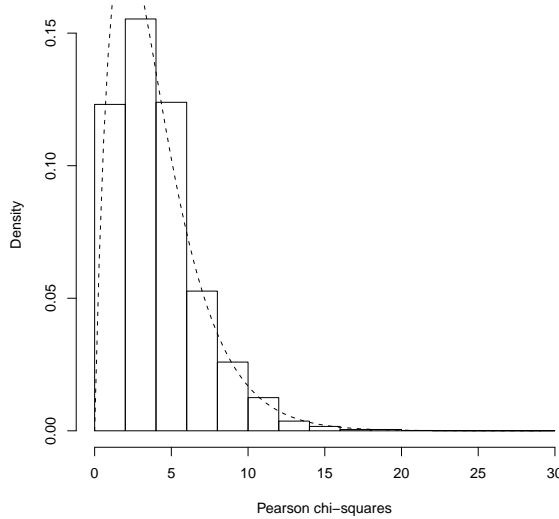


Figure 3: A histogram of sampled Pearson  $\chi^2$  goodness-of-fit for Table 1 generated by a Markov chain Monte Carlo method. The dotted curve is the corresponding asymptotic  $\chi_4^2$  distribution.

than or equal to the observed value  $\chi^2(\mathbf{x}^o) = 8.6687$ , then we have the estimate  $\hat{p} = 0.06681$ . Therefore we cannot reject  $H_0$  at significance level 0.05, which is the same result to the other strategies (a) and (b). Though the difference from the exact value  $p = 0.07035480$  from the simulated value is slightly larger than the asymptotic estimate ( $\hat{p} = 0.0699$ ), we may increase the accuracy of the estimates by increasing the sample sizes. To compare the three strategies for Table 1, we compute the upper percentiles of 90%, 95%, 99%, 99.9% for (a) asymptotic  $\chi_4^2$  distribution, (b) exact conditional distribution and (c) Monte Carlo simulated distribution in Table 3.

Finally, we give an example for which the structure of the Markov basis is complicated. The model we consider is a *no three-factor interaction model* for three-way contingency tables. The parametric description of the no three-factor interaction model is given by

$$\mathcal{M}_{n3} = \{\theta \in \Delta : \theta_{ijk} = \alpha_{ij}\beta_{ik}\gamma_{jk} \text{ for some } (\alpha_{ij}), (\beta_{ik}), (\gamma_{jk})\}.$$

This is one of the most important statistical models in the statistical data analysis of three-way contingency tables. The minimal sufficient statistics for  $\mathcal{M}_{n3}$  is the

Table 3: The upper percentiles for three strategies of Pearson goodness-of-fit  $\chi^2$  for Table 1.

	90%	95%	99%	99.9%
(a) Asymptotic $\chi_4^2$ distribution	7.779	9.488	13.28	18.47
(b) Exact null distribution	7.766	9.353	12.78	17.99
(c) Monte Carlo simulated distribution	7.684	9.287	12.73	18.58

two-dimensional marginals

$$\{x_{ij+}\}, \{x_{i+k}\}, \{x_{+jk}\},$$

where we define

$$x_{ij+} = \sum_{k=1}^K x_{ijk}, \quad x_{i+k} = \sum_{j=1}^J x_{ijk}, \quad x_{+jk} = \sum_{i=1}^I x_{ijk}.$$

We only consider  $3 \times 3 \times 3$  case (i.e.,  $I = J = K = 3$ ) here. Then the configuration matrix  $A$  is  $27 \times 27$  matrix written as follows.

$$A = \begin{pmatrix} 1 & 1 & 1 & 0 \\ 0 & 0 & 0 & 1 & 1 & 1 & 0 \\ & \\ & \\ 0 & 1 & 1 & 1 \\ 1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ & \\ & \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ & \\ & \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

For this model we see that the “simplest moves”, i.e., the moves with the minimum degree, correspond to the binomials of degree 4 such as

$$u_{111}u_{122}u_{212}u_{221} - u_{112}u_{121}u_{211}u_{222}, \quad (23)$$

which is called a *basic move*. There are 9 such moves for the case of  $3 \times 3 \times 3$  tables. Unfortunately, however, the set of these 9 moves does not become a Markov basis. To see this consider the following example.

**Example 2.6.** Consider the  $3 \times 3 \times 3$  contingency tables with the fixed two-dimensional marginals

$$(x_{ij+}) = (x_{i+k}) = (x_{+jk}) = (2, 1, 1, 1, 2, 1, 1, 1, 2)'. \quad (24)$$



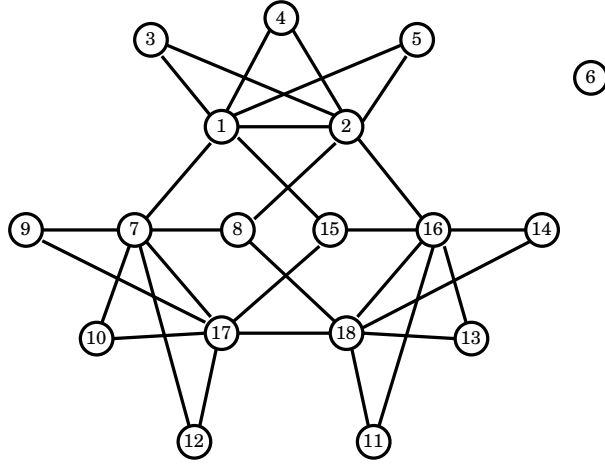


Figure 4: Undirected graph obtained from the set of the basic moves.

```

R = QQ[a11,a12,a13,a21,a22,a23,a31,a32,a33,
      b11,b12,b13,b21,b22,b23,b31,b32,b33,
      c11,c12,c13,c21,c22,c23,c31,c32,c33,
      x111,x112,x113,x121,x122,x123,x131,x132,x133,
      x211,x212,x213,x221,x222,x223,x231,x232,x233,
      x311,x312,x313,x321,x322,x323,x331,x332,x333,
      MonomialOrder=>{27,27}]
I = ideal(x111-a11*b11*c11,x112-a11*b12*c12,x113-a11*b13*c13,
      x121-a12*b11*c21,x122-a12*b12*c22,x123-a12*b13*c23,
      x131-a13*b11*c31,x132-a13*b12*c32,x133-a13*b13*c33,
      x211-a21*b21*c11,x212-a21*b22*c12,x213-a21*b23*c13,
      x221-a22*b21*c21,x222-a22*b22*c22,x223-a22*b23*c23,
      x231-a23*b21*c31,x232-a23*b22*c32,x233-a23*b23*c33,
      x311-a31*b31*c11,x312-a31*b32*c12,x313-a31*b33*c13,
      x321-a32*b31*c21,x322-a32*b32*c22,x323-a32*b33*c23,
      x331-a33*b31*c31,x332-a33*b32*c32,x333-a33*b33*c33)
G = gb(I); g = gens(G)
selectInSubring(1,g)

```

Unfortunately, this calculation may be hard to carry out for average PC. In fact, I could not finish the above calculation within one hour by my slow laptop (with 2.80 GHz CPU, 8.00 GB RAM, running on vmware). Instead, check the calculation for  $2 \times 3 \times 3$  cases. With the similar input commands, we have the output instantly in this case. From the output, we see that there are 1417 elements in the reduced Gröbner basis of  $I_A^*$ , and 15 elements in the reduced Gröbner basis of  $I_A$  as follows.

```

i10 : selectInSubring(1,g)

o10 = | x122x133x223x232-x123x132x222x233 x112x133x213x232-x113x132x212x233
-----
      x121x133x223x231-x123x131x221x233 x121x132x222x231-x122x131x221x232
-----
      x111x133x213x231-x113x131x211x233 x111x132x212x231-x112x131x211x232

```





```

0,0,0,1,0,0,0,0,0,0,0,0,0,1,0,0,0,0,0,0,0,0,0,1,0,0,0,0,0,0;
0,0,0,0,1,0,0,0,0,0,0,0,0,0,1,0,0,0,0,0,0,0,0,0,1,0,0,0,0,0;
0,0,0,0,0,1,0,0,0,0,0,0,0,0,0,1,0,0,0,0,0,0,0,0,0,1,0,0,0,0;
0,0,0,0,0,0,1,0,0,0,0,0,0,0,0,0,1,0,0,0,0,0,0,0,0,0,1,0,0,0;
0,0,0,0,0,0,0,1,0,0,0,0,0,0,0,0,0,1,0,0,0,0,0,0,0,0,0,1,0,0;
0,0,0,0,0,0,0,0,1,0,0,0,0,0,0,0,0,0,1,0,0,0,0,0,0,0,0,0,1,0;
0,0,0,0,0,0,0,0,0,1,0,0,0,0,0,0,0,0,0,1,0,0,0,0,0,0,0,0,0,1"
R = QQ[x111,x112,x113,x121,x122,x123,x131,x132,x133,
      x211,x212,x213,x221,x222,x223,x231,x232,x233,
      x311,x312,x313,x321,x322,x323,x331,x332,x333]
I = toricMarkov(A,R)

```

This calculation is finished within 1 second by my laptop. From the output, we see that 27 basic moves such as (23) and 54 moves of degree 6 such as (25) constitute a minimal Markov basis<sup>2</sup>. Using this minimal Markov basis, we can construct a connected Markov chain for this fiber. The corresponding undirected graph is Figure 5.

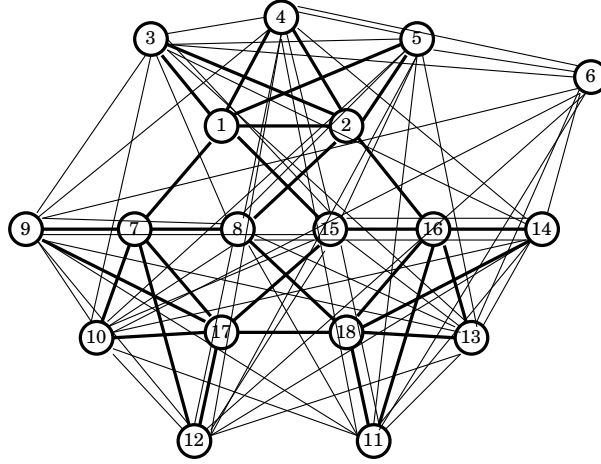


Figure 5: Undirected graph obtained from a minimal Markov basis.

Interestingly, for the problems of the larger sizes, the structure of the Markov basis becomes more complicated. For example, for the no three-factor interaction model of  $3 \times 3 \times 4$  tables, the set of degree 4, 6, 8 moves becomes a Markov basis, and for  $3 \times 3 \times 5$  tables, the set of degree 4, 6, 8, 10 moves becomes a Markov basis. These results are summarized in Chapter 9 of [3].

---

<sup>2</sup>The 4ti2 command `toricMarkov` gives a minimal Markov basis as the output. We can also obtain a Gröbner basis by the command `toricGroebner`.

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